A measure space approach to optimal source placement

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joint work with Eduardo Casas[2] and Karl Kunisch[1]

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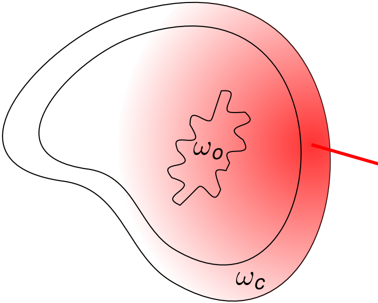
Motivation

- Optimization of light source locations in diffusive optical tomography
- Standard approach (discrete): combinatorial explosion with DOFs, requires initial set of feasible locations
- Here: Consider fictitious distributed "control field", apply sparse control techniques [Stadler '09] $\rightsquigarrow$ localization of sources
- Goal: Homogeneous illumination (application in photochemotherapy)



Sparse control problem

$$\begin{cases} \min_{u \in L^1(\omega_c)} \frac{1}{2} \|y - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{L^1(\omega_c)} \\ \text{subject to } Ay = \chi_{\omega_c} u, \quad y|_\Gamma = 0 \end{cases}$$

- ω_o, ω_c subdomains of $\Omega \subset \mathbb{R}^n$, $n = 2, 3$; $\Gamma := \partial\Omega$
- A linear elliptic operator
- $z \in L^\infty(\omega_o)$ given target
- L^1-type norms promote sparsity $\rightsquigarrow$ sparse controls
- Measure space required for well-posedness
  Alternative: control constraints
  [Stadler '09, D./G. Wachsmuth '11, Herzog/Casas/G. Wachsmuth]

Sparse control problem

$$\begin{cases} \min_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2} \|y - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} \\ \text{subject to } Ay = \chi_{\omega_c} u, \quad y|_\Gamma = 0 \end{cases}$$

- $\mathcal{M}_\Gamma(\overline{\omega}_c)$ Radon measures with compact support on $\overline{\omega}_c \setminus \Gamma$
- topological dual of $C_\Gamma(\overline{\omega}_c) = \{v \in C(\overline{\omega}_c) : v|_{\partial\omega_c \cap \Gamma} = 0\}$ ($\overline{\omega}_c \setminus \Gamma$ locally compact Hausdorff space)
- $\|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} = \sup_{\|\varphi\|_{C_\Gamma(\overline{\omega}_c)} \leq 1} \int \varphi \, du$

  $$(= \|u\|_{L^1(\omega_o)} \text{ for } u \in L^1(\omega_o))$$

- Partial observation requires primal-(pre)dual approach

Problem formulation

Assumption: adjoint A^* is isomorphism from $W_0^{1,q'}(\Omega)$ to $W^{-1,q'}(\Omega) := (W_0^{1,q'}(\Omega))^*$ for $q \in (1, \frac{n}{n-1})$ and $q' = \frac{q-1}{q} \in (n, \infty)$

Then: $W_0^{1,q'}(\Omega) \hookrightarrow C_0(\overline{\Omega})$, $\mathcal{M}(\Omega) \hookrightarrow W^{-1,q}(\Omega)$ compact,

- State equation $Ay = \mu$, $y|_\Gamma = 0$, has unique solution $y \in W_0^{1,q}(\Omega)$ for every $\mu \in \mathcal{M}(\Omega)$
- Control-to-state mapping (formal definition)

$$S_\omega : \mathcal{M}_\Gamma(\overline{\omega}_c) \to L^2(\omega_o), \qquad u \mapsto (A^{-1}(\chi_{\omega_c} u))|_{\omega_o}$$

is bounded linear operator, strongly continuous:

$$u_k \rightharpoonup^* u \text{ in } \mathcal{M}_\Gamma(\overline{\omega}_c) \quad \Rightarrow \quad S_\omega(u_k) \to S_\omega(u) \text{ in } L^2(\omega_o)$$

(smooth domain and coeff's; otherwise see [Meyer/Panizzi/Schiela '10])

Problem formulation

Control-to-state mapping

$$S_\omega : \mathcal{M}_\Gamma(\overline{\omega}_c) \to \mathrm{L}^2(\omega_o), \qquad u \mapsto (A^{-1}(\chi_{\omega_c} u))|_{\omega_o}$$

Reduced problem

$$(\mathcal{P}) \qquad \min_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2} \|S_\omega(u) - z\|^2_{\mathrm{L}^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)}$$

Existence of minimizer from standard arguments (weak-$\star$ topology on $\mathcal{M}_\Gamma(\overline{\omega}_c)$)

Optimality system

Introduce weak-$\star$ adjoint

$$S_\omega^\star : L^2(\omega_o) \to C_\Gamma(\overline{\omega}_c), \qquad \varphi \mapsto (A^{-*}(\chi_{\omega_o})\varphi)|_{\omega_c},$$

apply subdifferential calculus:

Theorem

Let $\overline{u} \in \mathcal{M}_\Gamma(\overline{\omega}_c)$ be a solution to $(\mathcal{P})$. Then there exists a $\overline{p} \in C_\Gamma(\overline{\omega}_c)$ satisfying

$$\text{(OS)} \qquad \begin{cases} S_\omega^\star(S_\omega(\overline{u}) - z) = \overline{p} \\ \langle \overline{u}, \overline{p} - p\rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \leq 0, \quad \|\overline{p}\|_{C_\Gamma(\overline{\omega}_c)} \leq \alpha \end{cases}$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ with $\|p\|_{C_\Gamma(\overline{\omega}_c)} \leq \alpha$.

Optimality system

Theorem

Let $\overline{u} \in \mathcal{M}_\Gamma(\overline{\omega}_c)$ be a solution to $(\mathcal{P})$. Then there exists a $\overline{p} \in C_\Gamma(\overline{\omega}_c)$ satisfying

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for all $p \in C_\Gamma(\overline{\omega}_c)$ with $\|p\|_{C_\Gamma(\overline{\omega}_c)} \le \alpha$.

$\rightsquigarrow$ sparsity of optimal control:

$$\operatorname{supp} \overline{u} \subset \{x \in \overline{\omega}_c : |\overline{p}(x)| = \alpha\}$$

Non-negative Controls

Control by light sources $\rightsquigarrow$ enforce non-negativity of controls

Problem

$$\min_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c),\, u \geq 0} \frac{1}{2} \|S_\omega(u) - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)}$$

Optimality system

$$(\mathrm{OS}_+) \qquad \begin{cases} S_\omega^\star(S_\omega(\overline{u}) - z) = \overline{p}, \\ \langle \overline{u}, \overline{p} - p \rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \leq 0, \qquad \overline{p} \geq -\alpha \end{cases}$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ with $p \geq -\alpha$.

Discretization

For simplicity: $\omega_o = \omega_c = \Omega$, shape-regular triangulation $\mathcal{T}_h$.

Finite element discretization of state:

$$Y_h := \left\{ y_h \in C_0(\overline{\Omega}) : \; y_h|_K \in P_1, K \in \mathcal{T}_h \right\}$$

Discrete state equation: $S_h : \mathcal{M}(\Omega) \to Y_h$, $u \mapsto y_h$,

$$a(y_h, v_h) = \int_\Omega v_h \, du \quad \text{for all } v_h \in Y_h.$$

Discretization

Discrete problem

$$(\mathcal{P}_h) \qquad \min_{u \in \mathcal{M}(\Omega)} \frac{1}{2} \|S_h(u) - z\|_{L^2(\Omega)}^2 + \alpha \|u\|_{\mathcal{M}(\Omega)}$$

- Control not discretized
  (cf. variational discretization of Hinze)
- $(\mathcal{P}_h)$ coercive and convex, but not strictly convex
- $\rightsquigarrow$ Solution exists, but is not unique

Discrete duality

Nodal basis $\{e_j\}_j$ of Y_h for interior nodes x_j:

$$y_h = \sum_j y_j e_j, \quad \text{where} \quad y_j = \langle y, \delta_{x_j} \rangle = y_h(x_j)$$

Dual of Y_h

$$D_h = \left\{ u_h \in \mathcal{M}(\Omega) : u_h = \sum_j \lambda_j \delta_{x_j}, \lambda_j \in \mathbb{R} \right\}$$

Projections

$$\Pi_h : C_0(\overline{\Omega}) \to Y_h, \quad \Pi_h y = \sum_j \langle y, \delta_{x_j} \rangle e_j$$

$$\Lambda_h : \mathcal{M}(\Omega) \to D_h, \quad \Lambda_h u = \sum_j \langle u, e_j \rangle \delta_{x_j}$$

Discrete duality

For all $u \in \mathcal{M}(\Omega)$, $v \in C_0(\overline{\Omega})$, $v_h \in Y_h$:

- $\langle u, v_h \rangle = \langle \Lambda_h u, v_h \rangle$ and $\langle u, \Pi_h v \rangle = \langle \Lambda_h u, v \rangle$
- $\|\Lambda_h u\|_{\mathcal{M}(\Omega)} \leq \|u\|_{\mathcal{M}(\Omega)}$,
- $\Lambda_h u \xrightharpoonup[h\to 0]{\star} u$ in $\mathcal{M}(\Omega)$ and $\|\Lambda_h u\|_{\mathcal{M}(\Omega)} \xrightarrow[h\to 0]{} \|u\|_{\mathcal{M}(\Omega)}$,
- $S_h(u) = S_h(\Lambda_h u)$

Theorem

- *$(\mathcal{P}_h)$ has unique solution $\overline{u}_h \in D_h$*
- *Any other solution $\tilde{u} \in \mathcal{M}(\Omega)$ satisfies $\Lambda_h \tilde{u} = \overline{u}_h$*

Convergence

Let:

- $\overline{u} \in \mathcal{M}(\Omega)$ solution of $(\mathcal{P})$ with state $\overline{y} = S(\overline{u})$,
- $\overline{u}_h \in D_h$ solution of $(\mathcal{P}_h)$ with state $\overline{y}_h = S_h(\overline{u}_h)$,

Theorem

- $\overline{u}_h \rightharpoonup^\star \overline{u}$ *in* $\mathcal{M}(\Omega)$ *and* $\|\overline{u}_h\|_{\mathcal{M}(\Omega)} \to \|\overline{u}\|_{\mathcal{M}(\Omega)}$
- $\|\overline{y} - \overline{y}_h\|_{L^2(\Omega)} \to 0$,
- $\frac{1}{2}\|\overline{y}_h - z\|^2_{L^2(\Omega)} + \alpha\|\overline{u}_h\|_{\mathcal{M}(\Omega)} \to \frac{1}{2}\|\overline{y} - z\|^2_{L^2(\Omega)} + \alpha\|\overline{u}\|_{\mathcal{M}(\Omega)}$

Numerical solution

For $u_h = \sum_j \lambda_j \delta_{x_j} \in D_h$,

$$\langle u_h, e_j \rangle = \lambda_j, \qquad \|u_h\|_{\mathcal{M}(\Omega)} = \sum_j |\lambda_j| = \|\lambda\|_1$$

$\rightsquigarrow$ reformulation in terms of λ_j, complementarity function:

Discrete optimality system

$$p_h = S_h^\star(S_h(u_h) - z)$$
$$\lambda_j = -\max(0, -\lambda_j + p_h(x_j) - \alpha) - \min(0, -\lambda_j + p_h(x_j) + \alpha)$$

semi-smooth in finite dimensions $\rightsquigarrow$ semi-smooth Newton method

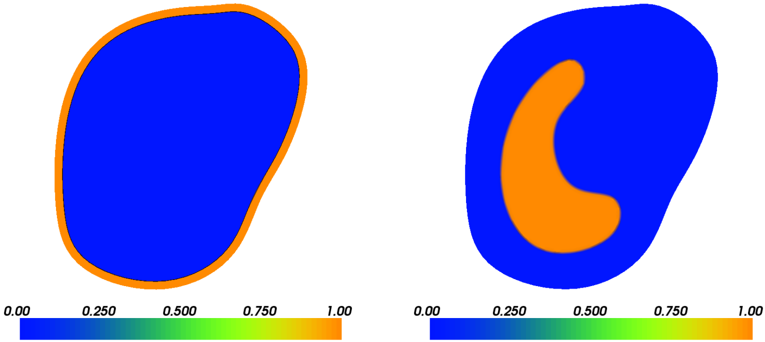
Model problem

$$\min_{y,u\geq 0} \frac{1}{2}\|y-z\|^2_{L^2(\omega_o)} + \alpha\|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)}$$

$$\text{s.t.} \begin{cases} -\nabla\cdot\left(\frac{1}{2(\mu_a+\mu_s)}\nabla y\right) + \mu_s y = \chi_{\omega_c} u & \text{on } \Omega, \\ \frac{1}{2(\mu_a+\mu_s)}\partial_\nu y + \rho y = 0 & \text{on } \partial\Omega \end{cases}$$

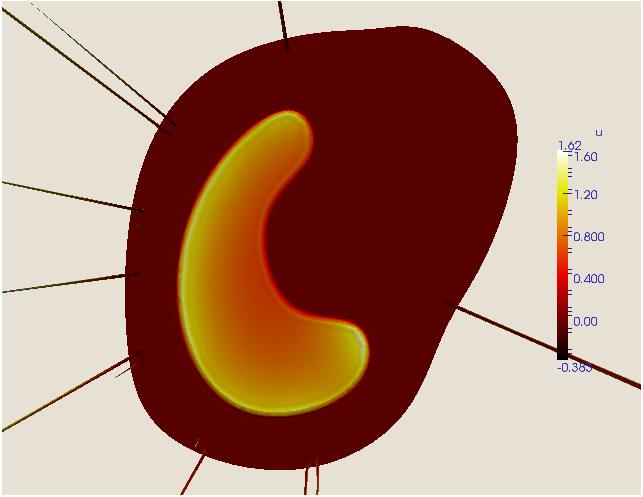
- describes diffusive light transport (e.g., in photochemotherapy)
- μ_a absorption coefficient, μ_s scattering coefficient, ρ reflection coefficient
- homogeneous illumination: $z \equiv 1$
- Finite element discretization in FEniCS

Example: Geometry

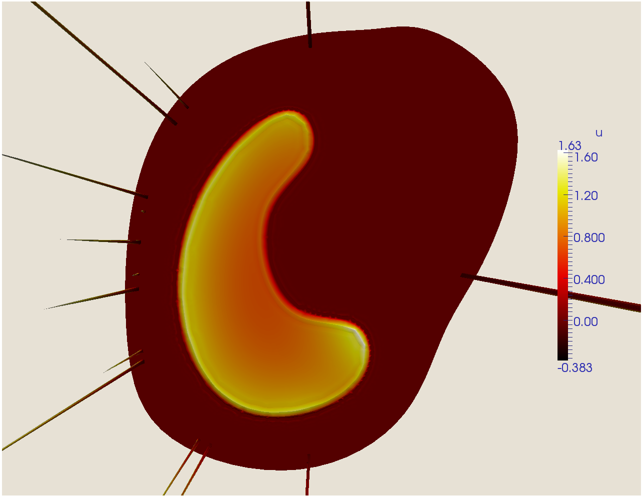


(a) control domain ω_c (b) observation domain ω_o

Example: $\alpha = 10^{-1}$



Example: $\alpha = 5 \cdot 10^{-2}$



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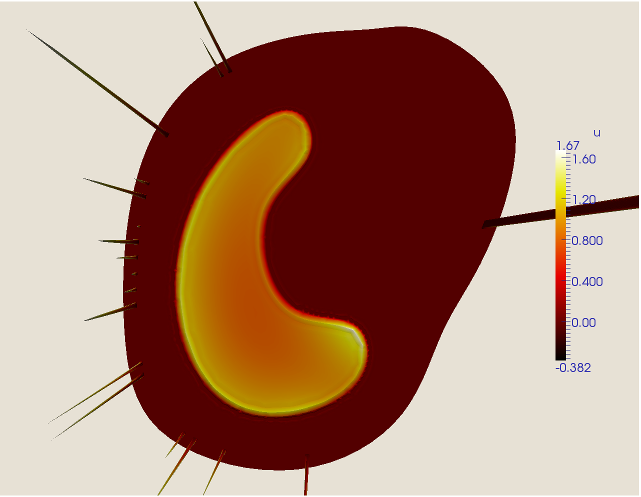
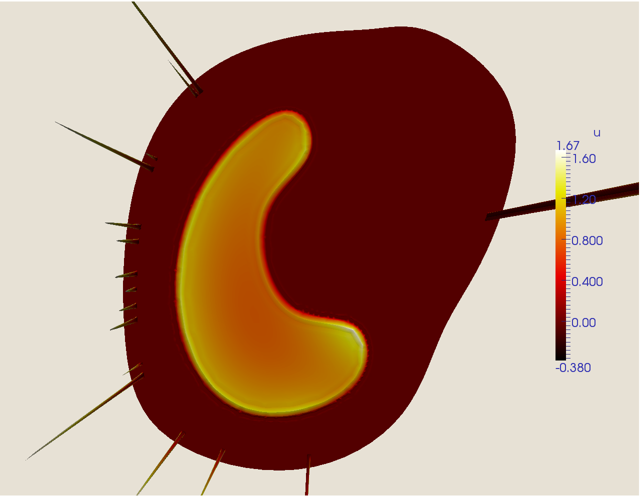


Example: $\alpha = 5 \cdot 10^{-3}$



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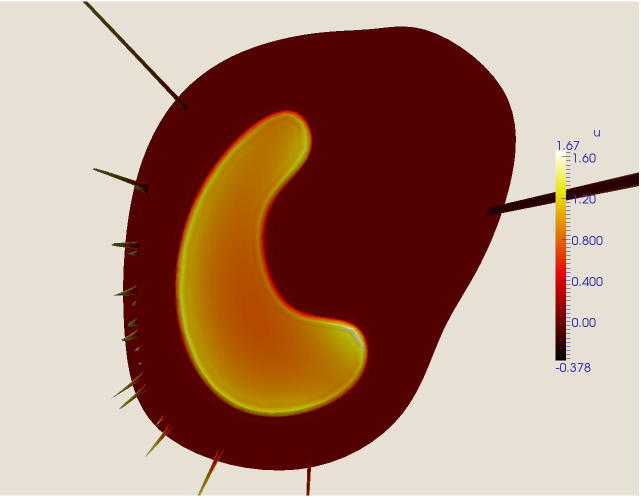
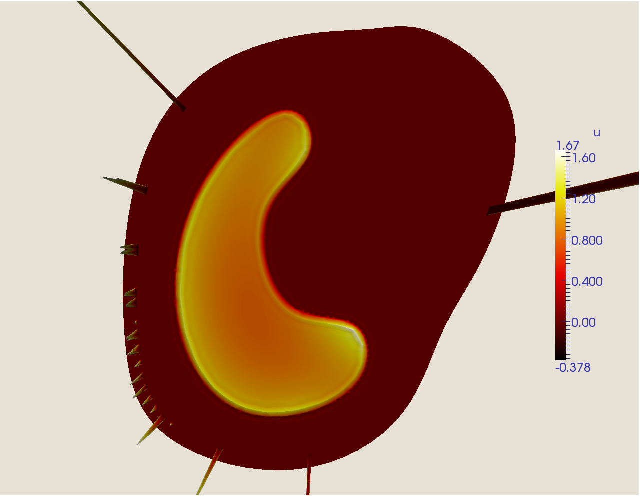
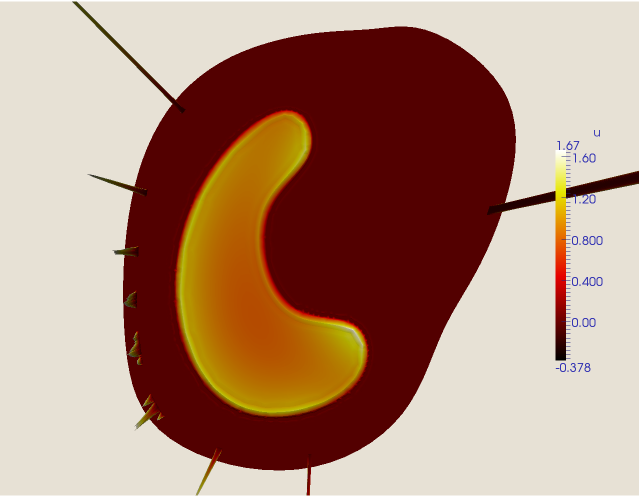


Example: $\alpha = 5 \cdot 10^{-4}$



Example: $\alpha = 10^{-4}$



Application to source placement

Measure space approach assumes

- Point sources
- Linear control costs

Not necessarily true in applications

$\rightsquigarrow$ decouple optimization of location and magnitude ("debiasing")

Application to source placement

Debiasing comparison:

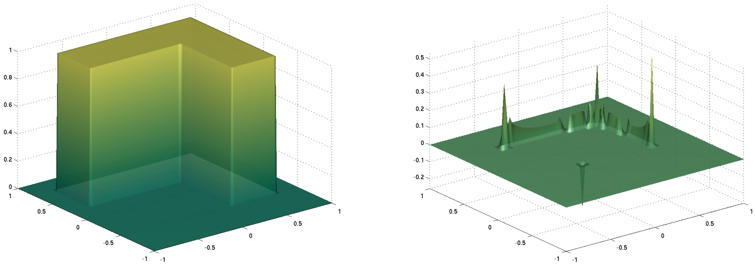
1. Solve measure space problem for large α (strong localization)
2. Select dominant "peaks", surrounding patches ω_i
3. Solve

$$\begin{cases} \min_{u\in\mathbb{R}^m} \frac{1}{2}\|y-z\|_{L^2(\Omega)}^2 + \frac{\beta}{2}|u|_2^2, \\ -\Delta y = \sum_{i=1}^m \chi_{\omega_i} u_i, \quad y|_\Gamma = 0 \end{cases}$$

   β chosen such that $|\overline{u}|_2 \approx M$ (given)

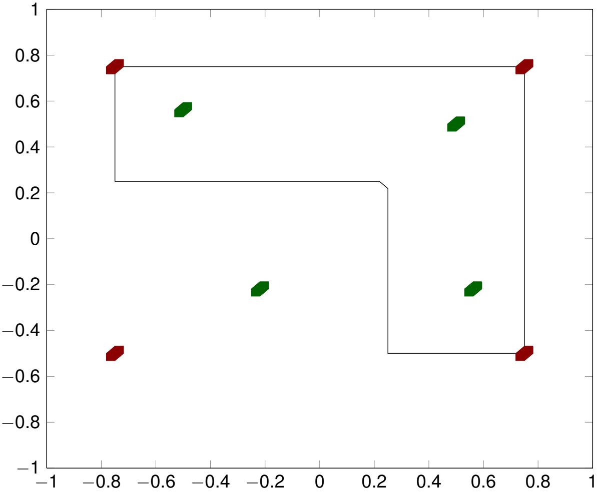
4. Repeat for heuristic patches (same area), same M
5. Compare tracking error $\|y^* - z\|_{L^2(\Omega)}$

Source placement: Geometry



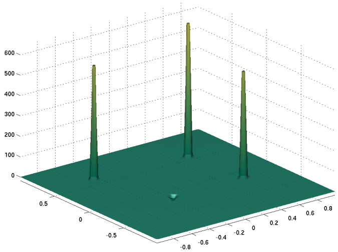
(a) target z (b) sparse control

Source placement: Control patches



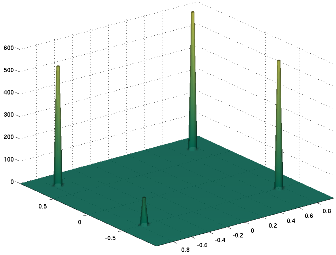
green: measure-based, red: heuristic

Source placement: Optimal controls



(a) measure-based

$\|\bar{y} - z\|_{L^2} \approx 0.44843$



(b) heuristic

$\|\bar{y} - z\|_{L^2} \approx 0.86210$

Conclusion

- Measure-space optimal controls are sparse
- Feasible technique for optimal source placement
- Natural discretization by linear combination of Dirac deltas
- Long-term goal: optimal experiment design in diffusive optical tomography

Cooperation partners:
Patricia Brunner, Manuel Freiberger, Hermann Scharfetter
(Institute of Medical Engineering, TU Graz)

Preprint, MATLAB code:
`http://www.uni-graz.at/~clason/publications.html`